Amendments to the Claims:

This listing of claims will replace all prior versions, and listings, of claims in the application:

Listing of Claims:

1. (currently amended) A computer implemented method to search a ~~heterogenous~~ heterogeneous compound database composed of molecules from different sources and syntheses, some known and some unknown, for molecules which are likely to have the same biological activity as a known query molecule comprising the following steps:

a) fragmenting a query molecule and database molecules according to a defined set of rules;

b) generating shape descriptors for the query molecule fragments and for the database molecules fragments; and

c) using the shape descriptors, comparing all combinations of query molecule fragments with database molecule fragments for each database molecule to identify ~~identifying~~ the database molecule which has a shape similar to the query molecule; and

d) outputting the identity of the database molecule.

2. (currently amended) A computer implemented method to search a heterogeneous ~~heterogenous~~ compound database composed of molecules from different sources and syntheses, some known and some unknown, for molecules which are likely to have the same biological

activity as a known query molecule comprising the following steps:

a) fragmenting a query molecule according to a defined set of rules;

b) topomerically aligning the query molecule fragments to generate a topomeric conformation;

c) generating the interaction energies between a probe and the atoms in the topomerically aligned query fragments at all intersection points in a three dimensional grid surrounding the aligned query fragments;

d) fragmenting a database molecule according to a defined set of rules;

e) topomerically aligning the database molecule fragments to generate a topomeric conformation;

f) generating the interaction energies between a probe and the atoms in the topomerically aligned database molecule fragments at all intersection points in a three dimensional grid surrounding the aligned database molecule fragments;

g) determining the similarity between query fragments and database molecule fragments by the root sum square differences in the field values; and

h) identify the molecule in the database most similar to the query molecule as that molecule having the smallest field value difference in its fragments; and

i) outputting the identity of the database molecule.

3. (currently amended) A computer implemented method to search a heterogeneous ~~heterogenous~~ compound database composed of molecules from different sources and syntheses,

some known and some unknown, for molecules which are likely to have the same biological activity as a known query molecule comprising the following steps:

a) fragmenting a query molecule according to a defined set of rules;

b) topomerically aligning the query molecule fragments to generate a topomeric conformation;

c) generating the interaction energies between a probe and the atoms in the topomerically aligned query fragments at all intersection points in a three dimensional grid surrounding the aligned query fragments;

d) assigning features locations in the topomerically aligned query fragments;

e) fragmenting a database molecule according to a defined set of rules;

f) topomerically aligning the database molecule fragments to generate a topomeric conformation;

g) generating the interaction energies between a probe and the atoms in the topomerically aligned database molecule fragments at all intersection points in a three dimensional grid surrounding the aligned database molecule fragments;

h) assigning features locations in the topomerically aligned database molecule fragments;

i) determining the similarity between query fragments and database molecule fragments by the root sum square differences in the field values;

j) identifying all database molecule fragments which have features, similarly located

in topomer space and similar in feature property, that match each feature in the query fragments; and

k) identifying the molecule in the database most similar to the query molecule as that molecule having the smallest field value difference in its fragments and smallest difference in features molecule; and

d) outputting the identity of the database molecule.

4. (previously presented) The method of claim 3 in which the feature contributions are weighted.

5. (previously presented) The method of claim 3 in which only hydrogen-bond-donating and hydrogen-bond-accepting features are used.

6. (currently amended) A computer implemented method to search a heterogeneous ~~heterogenous~~ compound database composed of molecules from different sources and syntheses, some known and some unknown, for molecular cores which are likely to have the same biological activity as a known query molecule core comprising the following steps:

a) specifying a known core and its two attachment bonds;

b) topomerically aligning the query core to generate a topomeric conformation;

c) generating the interaction energies between a probe and the atoms in the topomerically aligned query core at all intersection points in a three dimensional grid surrounding the aligned query core;

d) fragmenting database molecules into three fragments according to a defined set of

rules;

e) topomerically aligning the central database molecule fragments generated by the fragmentation process of step (d) to generate a topomeric conformation;

f) generating the interaction energies between a probe and the atoms in the topomerically aligned central database molecule fragments at all intersection points in a three dimensional grid surrounding the aligned central fragments;

g) determining the similarity between query core and central database molecule fragments by the root sum square differences in the field values; and

h) identifying the core in the database most similar to the query molecule core as that core having the smallest field value difference molecule; and

d) outputting the identity of the core.

7. (previously presented) The method of claim 6 in which an attachment penalty multiplier is employed.

8. (new) The method of claim 1 in which the output displays the fragment of the best hits and the query fragment that it matches.

9. (new) The method of claim 2 in which the output displays the fragment of the best hits and the query fragment that it matches.

10. (new) The method of claim 3 in which the output displays the fragment of the best hits and the query fragment that it matches.

11. (new) The method of claim 4 in which the output displays the fragment of the best hits

and the query fragment that it matches.

12. (new) The method of claim 5 in which the output displays the fragment of the best hits and the query fragment that it matches.

13. (new) The method of claim 6 in which the output displays the fragment of the best hits and the query fragment that it matches.

14. (new) The method of claim 7 in which the output displays the fragment of the best hits and the query fragment that it matches.